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Crystal Structures and Infrared Spectra of Two Fe-bearing Hydrous Magnesium Silicates Synthesized at High Temperature and Pressure

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Beamline(s): U2A

Introduction: Dense hydrous magnesium silicates (DHMS) synthesized at high temperatures and pressures have attracted much attention recently because of their potential role as major carriers for H and/or H2O in the subducting slabs and the Earth's mantle. Several DHMS has been synthesized in the MgO-SiO2-H2O system in the temperature-pressure range of 10-18 GPa and 600-1100 °C and designated as phases A, B, C, D, and E. While these DHMS have been widely studied structurally, little is known about the effects of Fe on the crystal chemistry and stabilities of these phases.

Methods and Materials: Two Fe-bearing hydrous magnesium silicates, Fe-bearing phase E with the composition $Mg_{2.22}Fe_{0.52}Si_{0.98}O_6H_{2.08}$, and phase E' with the composition $Mg_{2.13}Fe_{0.59}Si_{0.87}O_6H_{2.52}$, were synthesized in one charge in a multi-anvil apparatus at 14 GPa and 1400 °C for 47 hours and studied with single-crystal X-ray diffraction at the Geophysical Laboratory and infrared spectroscopy at U2A beamline at NSLS.

Results: The space groups and unit-cell parameters are $R\bar{3}m$, a = 2.981(1) Å, c = 13.898(3) Å for Fe-bearing phase E, and $P6_3/mmc$, a = 2.953(1) Å, c = 14.170(1) Å for phase E'. The structures of Fe-bearing phase E and phase E' are similar in many aspects, but they exhibit obvious differences in the stacking sequence of close-packed oxygen atoms, the distributions of M (=Fe+Mg) and Si cations between layers of close packed oxygen atoms, and the degree of the M cation ordering. The IR absorption spectra measured for phase E, Fe-bearing phase E, and E' are very comparable (Fig. 1). There are two very broad bands between 3000 and 3700 cm^{-1} with tails toward the low frequency and three intense bands below 1000 cm^{-1} for all samples. The broad bands in the principal OH-stretching region are due to either H_2O or weakly bonded OH, or both, indicating that the hydrogen atoms could be highly delocalized. The intense bands observed below 1000 cm^{-1} are attributed to Si-O stretching vibrations of the isolated SiO_4 tetrahedra. Interestingly, there is a systematic shift for all bands below 1000 cm^{-1} toward lower frequency from phase E to phase E', except for the lowest frequency mode around 800 cm^{-1}. This band shift could be related to the increase in the average Si-O bond distance from phase E to phase E'. In addition, the bands below 1000 cm^{-1} become increasingly more overlapped from phase E to phase E'. This observation is possibly associated with the substitution of Fe^{3+} for Mg^{2+} and the different structural symmetry, which is higher for phase E' than for phase E.

Conclusions: The synthesis and characterization of Fe-bearing phase E and phase E' demonstrate that the phase E-type structures can be rather compliant and complex, and that as we further explore the temperature-pressure-composition space, other types of structures that are similar to or related to the structure of phase E may be discovered.

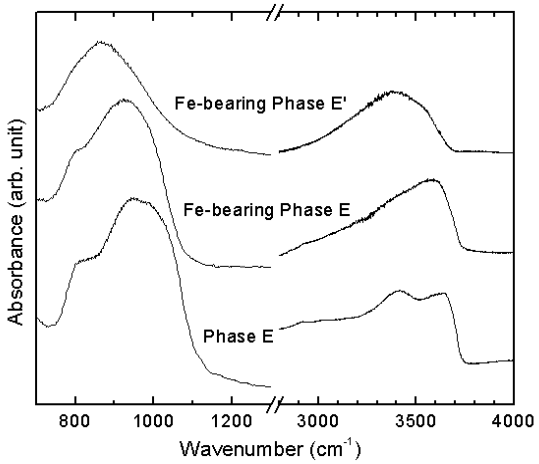

Fig. 1. Synchrotron IR absorption spectra of phase E, Fe-bearing phase E and phase E'.